accuracy of the simulation of the small-scale motions. It is clear that the dissipation rate is more accurately captured by the fixed-parameter multiscale model than by the original (non-multiscale) dynamic model, and that the dynamic multiscale model provides yet a further improvement in accuracy. The large initial error in the value as computed by the original dynamic model is quickly adjusted for by an overly large dissipation of the smallest resolved eddies, which reduces the dissipation rate to more nearly correct values at the cost of

less accurate simulation of those eddies. The multiscale models do not suffer from this large initial error and do not apply excessive dissipation to the small eddies. Later, as the flow evolves, the small eddies decay away, lessening the need for sub-grid-scale modeling; as a result, all methods become quite accurate.

Point of Contact: Alan Wray
(650) 604-6066
wray@nas.nasa.gov

Unstructured Large-Eddy Simulation Code for Simulation of Reacting Flows in Complex Geometries

K. Mahesh, G. Constantinescu, S. Apte, G. Iaccarino, P. Moin

A large-eddy simulation (LES) unstructured mesh code for high-fidelity simulation of turbulent reacting flows has been developed. The code is designed to run on massively parallel supercomputers. It can handle complex geometries and is being used to compute the flow and associated combustion phenomena in an industrial gas turbine combustor in collaboration with Pratt and Whitney (P&W). LES is chosen because of its demonstrated superiority in predicting turbulent mixing over Reynolds-averaged Navier-Stokes (RANS) formulation. Accurate simulations of chemically reacting flows are critically dependent on the ability to accurately simulate turbulent mixing.

The numerical algorithm allows for the use of hybrid grids. It is a conservative non-dissipative formulation—second-order accurate on uniform grids. The energy-conserving properties of the algorithm allow us to obtain a robust method without the need to introduce numerical dissipation, as is generally done in RANS codes. Keeping the numerical dissipation at

very low levels is essential to maintaining the accuracy of LES simulations. The code solves the incompressible flow equations or the low-Mach-number variable-density equations, the latter being used in simulations of reacting flows.

The dynamic LES model developed at the Center for Turbulence Research (CTR) is used to represent the subgrid stresses. The dynamic formulation offers many advantages when used in unstructured grid formulations, including dynamically computing the model coefficient (no empirical constants), eliminating the need for damping functions near solid surfaces, and eliminating the need for computing the distance to the wall.

Considerable effort was devoted to making the design of the code efficient. The code is fully parallel and uses Message Passing Interface. A novel algorithm was developed for grid-ordering, with the aim of minimizing processsor-to-processor communication. The code was ported to several platforms (e.g., Origin2000, IBM SP2, ASCI RED-Intel) and was

shown to scale well for computations using hundreds of processors, provided that the grid partition is such that each processor partition contains at least 5,000 nodes.

Validation simulations in the combustor geometry (a 1/18-combustor sector corresponding to one injector) provided by P&W are under way (see fig. 1). In particular, a special

P&W cold-flow combustor rig, for which detailed experimental data are available, will serve as the key validation test for complex geometries.

Point of Contact: Parviz Moin
(650) 604-5127
moin@rft33.nas.nasa.gov
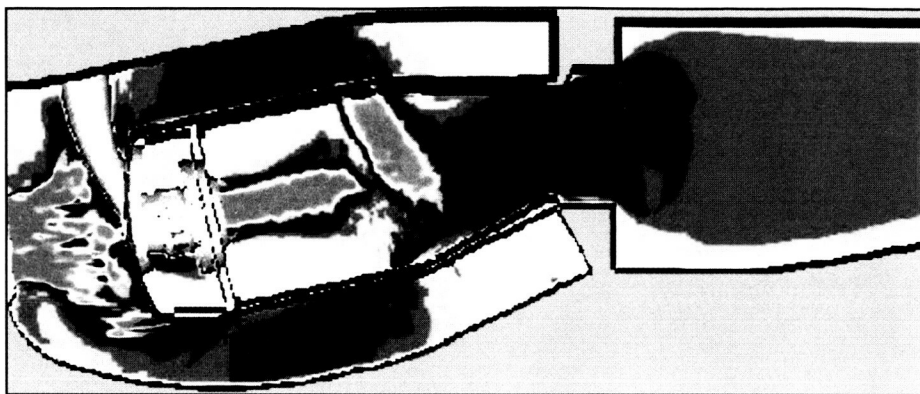
Fig. 1. Section through the PW6000 combustor (plane cutting through the injector symmetry plane). The simulation shows a 20-degree sector of the combustor that corresponds to one injector. Periodic boundary conditions are used on the lateral walls. Reynolds number based on the diffuser inlet section is Re = 36,000. The figure shows contours of velocity magnitude. The color scale is 0 (white) to 400 feet per second (dark blue), 40 contours. The results are from a 1.2-million node simulation. The grid is hybrid combination of tets, hexes, and pyramids.

Physics and Models for Optoelectronics Simulation

J. Li, S. H. Cheung, C. Z. Ning

Semiconductor optoelectronics delivers an integrated, reliable, and ultrafast solution to the ever-increasing bandwidth demand in information technology (IT). The objective of the current project at Ames Research Center is to develop the capability from first principles of physics to understand, design, and optimize optoelectronic devices, in order to meet the IT needs of NASA and the public. The project posted significant accomplishments in the area of comprehensive semiconductor laser simulation in FY00.

The research has increased knowledge across several fronts by (1) studying in more detail the role of many-body effects, or Coulomb interaction between charged carriers, in a semiconductor laser device; (2) clarifying the role of plasma heating in the operations of lasing devices; and, more important, (3) developing a hydrodynamic model for spatial inhomogeneous semiconductor lasers from first principles of microscopic physics.

Specifically, the following results were achieved. First, the researchers found that a